



46 As a consequence of the complex microstructure, the creep rate is controlled by a  
47 broad spectrum of simultaneously active deformation mechanisms. Indeed, during  
48 thermal creep, plastic strain is likely to result from the activation of both diffusion  
49 creep and dislocation motion. The relative contribution of each depends on the  
50 imposed stress state, on the internal stress state and on temperature. Vacancy driven  
51 diffusion creep processes, such as the Nabarro-Herring creep and Coble creep, tend to  
52 play an important role in the high-temperature regime [13,18]. Shrestha et al. [13]  
53 show that diffusion creep is dominant in modified 9Cr-1Mo steel at 873K (600°C)  
54 with a creep stress lower than 60 MPa. General Ashby's deformation map indicates  
55 that dislocation motion becomes the dominant mechanism under lower temperature  
56 and higher stress conditions. Clearly in the dislocation creep regime, the interaction  
57 between moving dislocations and precipitates, subgrain boundaries, and other  
58 dislocations will be dominant. Interestingly and on the basis of one dimensional  
59 models applied at the scale of the polycrystal the processes allowing to overcome  
60 obstacles (e.g. cross-slip, climb, unzipping) are expected to exhibit distinct  
61 temperature and stress dependence [19–22]. This warrants the existence of different  
62 creep regimes each controlled by a different process. Finally, as dislocations interact  
63 with subgrain boundaries and as different species migrate, both precipitate coarsening  
64 and subgrain growth can be also activated [2,6,17,23,24].

65 Polycrystal models can unravel the relative contribution of all dissipative  
66 processes. In an early work, Estrin and Mecking [25] developed a constitutive model  
67 assuming the average dislocation density is the sole structure factor affecting the  
68 mechanical state of the material. This model, which is a unified description for both  
69 dynamic loading and creep tests, tracks the dislocation density evolution through the  
70 Kocks-Mecking law and a kinetic equation is proposed to determine the flow stress  
71 and strain rate. Gottstein and Argon [26] treat the dislocation density evolution in a  
72 more sophisticated way. The dislocation glide, climb and cell wall migration are  
73 considered in the dislocation storage and dynamic recovery processes. Roters et al.  
74 [27] divided the dislocations in the cell-forming materials into three subsets: mobile  
75 and immobile dislocations within the subgrain, and immobile dislocations in the cell  
76 wall. An evolution law is proposed for each population taking into account the  
77 dislocation dipole and lock formation. While the aforementioned models focused  
78 mainly on the frameworks to track the evolution of dislocation populations, other  
79 body of work focuses on the details of the dislocation/obstacle bypass processes, i.e.  
80 [19,21,28,29]. Xiang and Srolovitz [28] performed dislocation dynamic simulations  
81 on this subject for both penetrable and impenetrable particles, with dislocation glide,  
82 climb and cross-slip mechanisms included. The climb velocity for the edge  
83 dislocation was determined through the climb component of Peach-Koehler force. The  
84 results show that generally the climb mechanism tends to reduce the stress required  
85 for the bypass.

86 The present work proposes a physics-based constitutive model, capable of  
87 simultaneously predicting the mechanical response of high Cr steels and of evaluating  
88 the contribution of each mechanism during thermal creep. In this crystal plasticity  
89 based model, thermally activated dislocation glide and climb mechanisms are coupled.  
90 Their activation rates are determined via the use of harmonic transition state theory  
91 based framework. Further, we propose to predict the activation of climb and explicit  
92 treatment of vacancy flux towards dislocations. The model presented, uses a recently  
93 proposed framework, to account for the distribution of internal stresses at a  
94 sub-material point scale. This added feature also allows selectively activating distinct

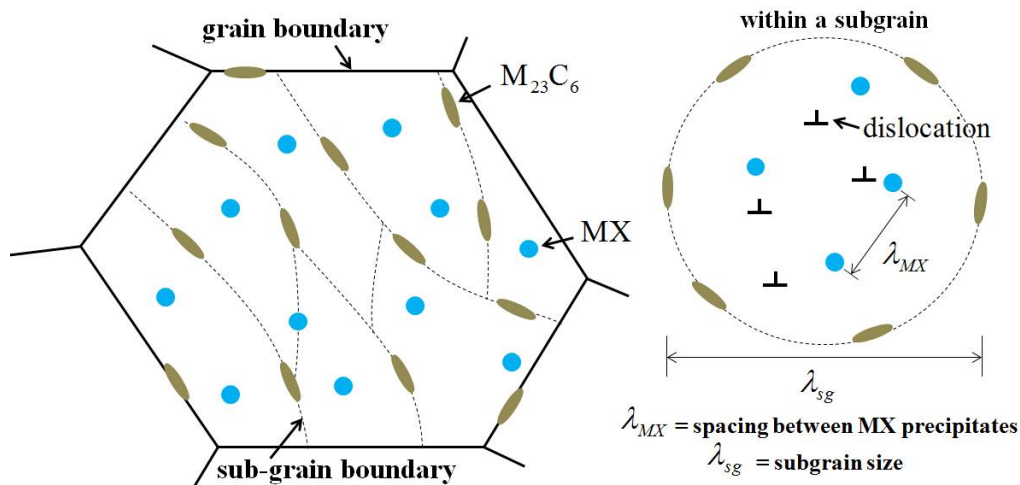
95 dislocation glide and recovery processes (i.e. dislocation annihilation within subgrains  
 96 and in subgrain boundaries). The constitutive law is embedded in a mean-field  
 97 visco-plastic framework (VPSC) [30,31]. The model is employed to predict the  
 98 behavior of the modified 9Cr-1Mo alloy under thermal creep tests at various  
 99 temperatures and stresses. The predicted results are in a fairly good agreement with  
 100 the experimental data. Among others, it is suggested that dislocation recovery within  
 101 the subgrain could play a dominant role in the strain rate evolution observed during  
 102 creep tests.

103 The study is structured as follows. A detailed description of the proposed thermal  
 104 creep model will be given in Section 2 including the modeling background, the  
 105 formulation to determine the creep shear rate on each slip system and a brief  
 106 introduction of the VPSC framework. In Section 3, the predicted thermal creep  
 107 responses are presented and compared with the experimental data provided by Basirat  
 108 et al. [14] for Fe-9Cr-1Mo steel under various temperatures and applied stresses. The  
 109 studies on the contributions of the mechanisms and the parameter sensitivities are also  
 110 proposed. Section 4 presents a discussion of the role of each dislocation recovery  
 111 process on the stress dependence of the creep rate.

## 112 2 Modeling framework

### 113 2.1 Microstructure and considered mechanisms

114 A paradigm microstructure, with features characteristic of high Cr alloys  
 115 schematically presented in Fig.1, is chosen as the foundation of this model. This is the  
 116 typical microstructure for heat treated and thermo-mechanically processed high Cr  
 117 steels [1,3,6,13]. As shown, each grain contains a number of elongated subgrains  
 118 which boundaries are denoted with dotted lines. Each subgrain contains a high density  
 119 of dislocations ( $\sim 10^{14} \text{ m}^{-2}$ ). Within subgrains quasi-spherical MX precipitates are  
 120 considered to be randomly dispersed. According to Refs [6,32], the average size of  
 121 MX particles is around 20-50 nm, with mean inter-spacing in the order of 300 nm.  
 122 Larger rod-like  $M_{23}C_6$  precipitates (100-300 nm) are located mainly in the grain and  
 123 subgrain boundaries.



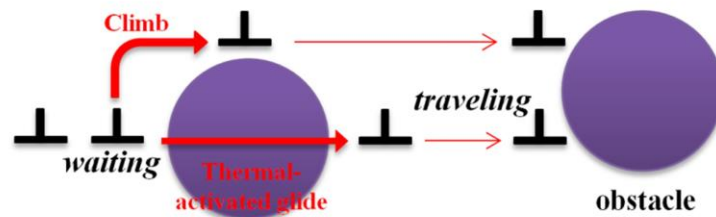
124

125

Fig.1. Schematic view of the microstructure for heat treated high Cr steels.

126 With this microstructure and given the moderate stress range considered in this  
 127 study, it is foreseen that dislocation motion is arrested at subgrain boundaries (cell  
 128 walls) and that dislocation transmission across the boundary is unlikely. Recall here  
 129 that these boundaries contain non-shearable precipitates. In this work, the dislocations  
 130 are divided into two subsets: subgrain interior dislocations and cell wall dislocations.  
 131 Plastic deformation is controlled by dislocation glide within subgrains. Those  
 132 dislocations may be mobilized or immobilized depending on the local stress state and  
 133 defect content (see section 2.2). Importantly, one notes that subgrains are expected to  
 134 have a complex stress state due to the dislocations and precipitates they contain. One  
 135 therefore expects cell walls to exhibit a long-range stress field arising from the  
 136 primary dislocation network and rod-like precipitates within the subgrain boundaries.

137 Within subgrains, two types of obstacles to dislocation motion are considered:  
 138 MX precipitates and other dislocations within the cell. The effective dislocation  
 139 mobility is determined by their waiting time at both types of obstacles. Stored  
 140 dislocations can overcome MX precipitates via either a thermally activated glide  
 141 (junction unzipping and Orowan bypass mechanism for incoherent precipitates) or a  
 142 climb assisted glide process depicted in Fig. 2. The climb process is non-conservative  
 143 and therefore is rate limited by the vacancy flux towards or away from the dislocation  
 144 [19–22].



145  
 146 Fig. 2. Schematic view of the obstacle-bypass mechanisms for moving dislocations.

147 The evolution of the dislocation population within the subgrain is complex as the  
 148 following processes are simultaneously active: (i) dislocation generation; (ii) dynamic  
 149 recovery resulting from the short range interaction with other dislocations; (iii)  
 150 trapping in the subgrain boundaries. The dislocations population in the cell wall can  
 151 also reconfigure itself with time. It is postulated here that within cell walls  
 152 annihilation due to climb is a dominant feature. Rigorously, the dislocation  
 153 annihilation in the cell wall should result in a change in the subgrain size, and hence  
 154 affect the mechanical response [33,34]. However, this process is not considered here  
 155 due to the lack of related statistical information. In addition, within the temperature  
 156 and stress regimes considered (873K (600°C)-973K (700°C),  $\geq 80$  MPa), diffusion  
 157 creep and precipitate coarsening are neglected.

158  
 159 **2.2 Constitutive law**

160 The proposed model deals with the mechanical behavior at material point level.  
 161 Within the paradigm microstructure, a material point will represent a grain containing  
 162 a number of subgrains. The stress distribution within a material point is heterogeneous.

163 Theoretically, each material point can be decomposed into infinite sub-material points.  
 164 The stress state is different at each point depending on the local dislocation  
 165 arrangement. Some dislocations within the subgrain may be able to overcome the  
 166 obstacles and keep gliding, whereas others will be immobilized due to the low stress  
 167 state acting on them. However, effective medium models such as the VPSC model  
 168 used in this work determine the inclusion-matrix interaction assuming the state inside  
 169 of the grain or grain cluster is homogenous. Thus, it is necessary to properly express  
 170 the mean mechanical behavior considering the response in all sub-material points.

171 Using a crystal plasticity formalism, the plastic strain rate at the material point  
 172 scale can be written as the sum of the shear strain rates on all potentially active slip  
 173 systems as follows:

$$174 \quad \dot{\epsilon}_{ij}^p = \sum_s m_{ij}^s \bar{\gamma}^s \quad (1)$$

175 Here  $m_{ij}^s = \frac{1}{2}(n_i^s b_j^s + n_j^s b_i^s)$  is the symmetric Schmid tensor associated with slip  
 176 system  $s$  in a material point  $p$ ;  $\mathbf{n}^s$  and  $\mathbf{b}^s$  are the normal and Burgers vectors of  
 177 this system.  $\bar{\gamma}^s$  denotes the mean shear rate in one material point. Similarly to the  
 178 approach proposed in [35,36] the latter is given by an integral over all the local shear  
 179 rates weighted by the volume fraction of the sub-material point. In the calculation, a  
 180 probability distribution function  $P$  is used to represent the volume fraction  
 181 distribution of sub-material points with a resolved shear stress ( $\tau^s$ ).  $P$  is referred to  
 182 the average resolved shear of the material point ( $\bar{\tau}^s$ ):

$$183 \quad \bar{\gamma}^s = \int_{-\infty}^{\infty} \dot{\gamma}^s(\tau^s) P(\tau^s - \bar{\tau}^s) d\tau^s \quad (2)$$

184 where  $\bar{\tau}^s = \boldsymbol{\sigma} : \mathbf{m}$  with  $\boldsymbol{\sigma}$  being the deviatoric stress of the material point.  $\dot{\gamma}^s$   
 185 represents the shear rate of a sub-material point.  $P$  is described by the Gaussian  
 186 distribution function:

$$187 \quad P(\tau^s - \bar{\tau}^s) = \frac{1}{\sqrt{2\pi V}} \exp\left(-\frac{(\tau^s - \bar{\tau}^s)^2}{2V}\right) \quad (3)$$

188  $V$  is the variance of the resolved shear stress, which is linked to the dislocation density  
 189 [35,36]. It should be different for each slip system and vary during the deformation.  
 190 However, for the sake of simplicity, we assume  $V$  is equal for all systems since the  
 191 initial dislocation arrangement is not completely known. Moreover,  $V$  is considered as  
 192 constant throughout the creep tests. The decrease of dislocation density during creep  
 193 will lead to a lower  $V$  value, and hence will further reduce the shear rate. However,  
 194 this effect is out of the scope of the present work. In the proposed model, the creep  
 195 strain is accumulated due to the motion of the dislocations in the interior of the  
 196 subgrains. The shear rate at each sub-material point can be expressed by the Orowan's  
 197 equation as:

$$198 \quad \dot{\gamma}^s = \rho_{cell}^s b v^s \cdot \text{sign}(\bar{\tau}^s) \quad (4)$$

199 where  $\rho_{cell}^s$  is the density of dislocations within the subgrains.  $b$  is the magnitude

200 of the Burgers vector, and  $v^s$  is the mean velocity of dislocations traveling between  
 201 obstacles. The mean dislocation velocity is given by the dislocation mean free path  
 202 between obstacles  $\lambda^s$ , divided the time spent in this process. The latter includes the  
 203 time traveling between obstacles  $t_t^s$  and the average time a dislocation spends  
 204 waiting at an obstacle  $t_w^s$  [37–39]:

$$205 \quad v^s = \frac{\lambda^s}{t_t^s + t_w^s} \quad (5)$$

206 The presence of multiple types of obstacles leads to a reduction in the mean free path.  
 207 Here choice is made to express  $\lambda^s$  as the geometric mean of the interspacing for  
 208 individual obstacles:

$$209 \quad \frac{1}{\lambda^s} = \frac{1}{\lambda_{\rho,cell}^s} + \frac{1}{\lambda_{MX}^s} \quad (6)$$

210 with  $\lambda_{\rho,cell}^s$  and  $\lambda_{MX}^s$  denote the dislocation mean free path for dislocation obstacles  
 211 and MX precipitates, respectively. The obstacle interspacing determination depends  
 212 on the nature of the barrier. To first order,  $\lambda_{\rho,cell}^s$  is inversely proportional to the  
 213 hardening contribution of the dislocations in the cell, as  $\tau_{\rho,cell}^s \propto \mu b / \lambda_{\rho,cell}^s$ . To  
 214 describe the latent hardening associated with dislocation-dislocation interactions  
 215 between slip systems, the law proposed by Franciosi and Zaoui [40], and for which  
 216 discrete dislocation dynamics simulations have demonstrated the statistical  
 217 representativeness [41] is used in this work as:

$$218 \quad \tau_{\rho,cell}^s = \mu b \sqrt{\sum_s \alpha^{ss'} \rho_{cell}^{s'}}$$

219 Also one has:

$$220 \quad \frac{1}{\lambda_{\rho,cell}^s} = \sqrt{\sum_s \alpha^{ss'} \rho_{cell}^{s'}}$$

221  $\alpha^{ss'}$  is the effective latent hardening matrix. The interspacing for MX precipitates is  
 222 written in a simple form derived from the geometrical configuration of the obstacles  
 223 on the slip plane [22,42,43].

$$224 \quad \frac{1}{\lambda_{MX}^s} = h_{MX} \sqrt{N_{MX} d_{MX}} \quad (9)$$

225 here  $h_{MX}$  is the trapping coefficient for MX precipitate.  $N_{MX}$  and  $d_{MX}$  denote the  
 226 number density and size of MX precipitates. This law is appropriate for hard obstacles  
 227 [44], such as MX precipitates. Friedel [45] proposed an alternative expression for  
 228 attractive obstacles on the glide plane, which is more suitable for weak obstacles.

229 In Eq. 5 the traveling time is given by  $t_t^s = \lambda^s / v_t$ . Here  $v_t$  is the dislocation  
 230 traveling velocity which is assumed to be equal to the shear wave velocity  $C_s$   
 231 (independent of the driving force) since the traveling time is negligible compared to

232 the waiting time. It can be determined by  $v_t \approx C_s = \sqrt{\mu/\rho_0}$  [39,46] where  $\rho_0$  is the  
 233 mass density and  $\mu$  is the shear modulus given by  $\mu = 103572 \text{ MPa} - T \cdot 48 \text{ MPa/K}$  [47].

234 To determine the dislocation average waiting time, we define the theoretical  
 235 waiting times of thermally-activated glide ( $t_{w,g}$ ) and climb ( $t_{w,c}$ ). These two  
 236 mechanisms, however, occur simultaneously, which can effectively reduce the waiting  
 237 time. To first order the waiting time at the obstacle type  $i$  (other dislocations,  $i = \rho$   
 238 or MX precipitates,  $i = MX$ ) within a sub-material point can be expressed using the  
 239 harmonic mean:

$$240 \quad \frac{1}{t_{w,i}^s} = \frac{1}{t_{w,g,i}^s} + \frac{1}{t_{w,c,i}^s} \quad (10)$$

241 One notes here that a harmonic transition state theory based treatment could yield  
 242 more accurate estimates. The mean waiting time of slip system  $s$  when both  
 243 obstacles are considered is given by the average of  $t_{w,\rho}^s$  and  $t_{w,MX}^s$ , weighted by the  
 244 probability that the individual type of obstacle is encountered by the moving  
 245 dislocation:

$$246 \quad t_w^s = P_\rho t_{w,\rho}^s + (1 - P_\rho) t_{w,MX}^s \quad (11)$$

247  $P_\rho$  is the probability that a dislocation encounters other dislocation and  $1 - P_\rho$  that  
 248 it encounters MX precipitates. Statistically, the inverse of mean free path represents  
 249 the number of obstacles per unit length along the gliding direction. In this way, the  
 250 ratio of dislocation type obstacles in the corresponding section can be determined by  
 251 the proportion between  $1/\lambda_\rho^s$  and  $1/\lambda^s$ . Connecting with Eqs. 6-9, we will have:

$$252 \quad P_\rho = \frac{1/\lambda_\rho^s}{1/\lambda^s} = \frac{\sqrt{\sum_s \alpha^{ss'} \rho_{cell}^{s'}}}{\sqrt{\sum_s \alpha^{ss'} \rho_{cell}^{s'} + h_{MX} \sqrt{N_{MX} d_{MX}}}} \quad (12)$$

### 253 **2.2.1 Thermally-activated glide**

254 The thermally activated glide describes the obstacle bypass processes including  
 255 the unzipping of the junctions and the Orowan mechanism for large size particles. The  
 256 MX precipitates are incoherent with the matrix and therefore impenetrable. In this  
 257 case, the bypass at low-stress states is unlikely. However, under high driving stress,  
 258 the dislocation can bow out between the MX precipitates, merge on the other side of  
 259 the obstacle and continue to glide. The bypass for both types of obstacles can be  
 260 considered as thermally-activated process. Therefore,  $t_{w,g,MX}^s$  and  $t_{w,g,\rho}^s$  can be  
 261 described using the Kocks-type activation enthalpy law [37,39,48] but with different  
 262 values for the attempt frequencies and activation energies:

$$263 \quad \frac{1}{t_{w,g,i}^s} = \frac{v_{G,i}^s}{\exp\left(\frac{\Delta G_i^s}{kT}\right)} \quad (i = MX \text{ or } \rho) \quad (13)$$

264 In Eq. 13,  $i$  refers to different types of obstacles (dislocations or MX precipitates).

265  $\nu_{G,i}^s$ ,  $k$  and  $T$  are the effective attempt frequency, Boltzmann constant and  
 266 absolute temperature, respectively.  $\Delta G_i^s$  denotes the activation energy given by:

$$267 \quad \Delta G_i^s = \begin{cases} \Delta G_{0,i} \left( 1 - \left( \frac{|\tau^s|}{\tau_c^s} \right)^p \right)^q & \text{if } |\tau^s| < \tau_c^s \\ 0 & \text{if } |\tau^s| \geq \tau_c^s \end{cases} \quad (14)$$

268 where  $\Delta G_{0,i}$  is activation energy without any external stress applied. Its value is  
 269 dependent on the nature of the obstacle, such as the dislocation interaction and the  
 270 strength and size of precipitates.  $p$  ( $0 < p \leq 1$ ) and  $q$  ( $1 \leq q < 2$ ) are the  
 271 exponent parameters in the phenomenological relation determining the shape of the  
 272 obstacles resistance profile [48].  $\tau_c^s$  is the critical resolved shear stress (CRSS). The  
 273 hardening contributions from the dislocations in the subgrain and MX precipitates, as  
 274 well as the  $M_{23}C_6$  precipitates and the dislocations in the cell wall due to the long term  
 275 stress field. The long-range hardening induced by multiple sources has been studied in  
 276 many works i.e. [42,49,50]. A commonly used superposition principle is written as:

$$277 \quad \tau_i^m = \tau_1^m + \tau_2^m \quad (15)$$

278  $\tau_1$  and  $\tau_2$  are the hardening due to source 1 and 2, respectively.  $\tau_i$  denotes the  
 279 superimposed hardening. The exponent  $m$  varies between 1 and 2 depending on the  
 280 hardening mechanisms. A value higher than 2 is reported for irradiation-induced  
 281 defects [42]. The long range hardening sources within the microstructure paradigm  
 282 include the MX precipitates,  $M_{23}C_6$  carbides and the dislocations. Notice that the  
 283 dislocations comprise two populations: the ones within the subgrain cell ( $\rho_{cell}$ ) and  
 284 the ones in cell wall ( $\rho_{cw}$ ). Both of them contribute to the hardening due to the long  
 285 range stress field with similar features. Consequently, it is reasonable to consider them  
 286 as one individual hardening source. As mentioned above, the hardening due to  
 287 dislocation can be obtained using the complex form of the Taylor law:

$$288 \quad \tau_\rho^s = \mu b \sqrt{\sum_s \alpha^{s'} (\rho_{cell}^{s'} + \rho_{cw}^{s'})} \quad (16)$$

289 The precipitate hardening should superimpose with  $\tau_\rho^s$  using the principle in Eq. 15.  
 290 Moreover, the linear superimposition is restricted if one of the hardening sources is  
 291 the intrinsic frictional resistance  $\tau_0^s$  [42,49,50]. Therefore, the total CRSS is given  
 292 by:

$$293 \quad \tau_c^s = \tau_0^s + \left( (\tau_\rho^s)^m + (\tau_p^s)^m \right)^{1/m} \quad (17)$$

294  $\tau_p^s$  is the hardening contributions by both MX and  $M_{23}C_6$  precipitates.

295 In this work, the attempt frequency for overcoming an MX precipitate is assumed to  
 296 be constant. The one for junction unzipping process  $\nu_{G,\rho}$  is suggested to be  
 297 dependent on the dislocation traveling velocity, an entropy factor  $\chi$  (of the order of



298 1) and the average length of the vibrating dislocation segments (represented by the  
 299 dislocation mean free path  $\lambda^s$ ) [36,51].

$$300 \quad v_{G,\rho} = \chi C_s / \lambda^s \quad (18)$$

### 301 **2.2.2 Dislocation climb**

302 Dislocation climb refers to the process that edge dislocations migrate  
 303 perpendicular to the slip plane via point defect absorption/emission. This stress- and  
 304 temperature-dependent mechanism may assist the edge dislocations to bypass the  
 305 barriers during deformation. The effects of climb are more evident at  
 306 high-temperature due to the high concentration and diffusivity of point defects  
 307 [19–22]. In the present work, the concept of climb waiting time (Eq. 10) is introduced  
 308 to describe this process. Notice that the activation of climb process will affect the  
 309 mean dislocation mobility, but the sign of shear rate is only governed by the resolved  
 310 shear stress, which captures the fact that the climb mechanism is assisting the  
 311 dislocation glide.

312 Several modeling works have focused on the case of dislocation climb  
 313 [18,22,46,52–55]. From the physics standpoint, the climb velocity depends on the  
 314 climb driving force and on the flow of point defects into the edge dislocations. The  
 315 climb component of Peach-Koehler force has been discussed in Refs. [56–60] and is  
 316 essential to determine the climb rate on each slip system in a crystallographic  
 317 framework. Notice that climb may be a reaction-rate-controlled process or a  
 318 diffusion-controlled process [18]. The former usually occurs in irradiated materials,  
 319 where the current of defects entering and/or leaving the dislocation core are very large  
 320 and reach the defect-dislocation reaction rate limit. Otherwise, climb is a  
 321 diffusion-controlled process, such as in the thermal creep case. Some authors  
 322 [18,46,52–55] determine the flux of vacancies through the gradient of the vacancy  
 323 concentration in the dislocation control volume. The detailed description of this  
 324 method is given in the Appendix. The net current of vacancies  $I_v^s$  for slip system  $s$   
 325 can be expressed as:

$$326 \quad I_v^s = \frac{2\pi b D_v \left[ C_v^\infty - C_v^0 \exp\left(\frac{-f_c^s \Omega}{kTb}\right) \right]}{\Omega b \ln(r_\infty / r_d)} \quad (19)$$

327 here  $\Omega \approx b^3$  is the atomic volume.  $D_v$  is the vacancy diffusivity.  $C_v^0$  is the  
 328 equilibrium vacancy concentration at temperature  $T$  in the bulk of the crystal, given  
 329 by  $C_v^0 = \exp(S_f^v/k) \exp(-E_f^v/kT)$  [18].  $E_f^v$  and  $S_f^v$  are the vacancy formation  
 330 energy and entropy, respectively.  $C_v^\infty$  represents the vacancy concentration in the  
 331 material matrix which is assumed to be equal to  $C_v^0$  in the present work.  $f_c^s$  is the  
 332 climb component of Peach-Koehler force [56–60].  $r_d$  and  $r_\infty$  denote the radii of the  
 333 inner and outer boundaries for the cylindrical control volume defined around the  
 334 dislocation line. Therefore, the climb velocity is given by:

$$335 \quad v_c^s = \frac{I_v^s \Omega}{b} = \frac{2\pi D_v \left[ C_v^\infty - C_v^0 \exp\left(\frac{-f_c^s \Omega}{kTb}\right) \right]}{b \ln(r_\infty / r_d)} \quad (20)$$

336 The waiting time for climb can be determined by the ratio between the mean  
 337 climb velocity of the edge dislocation and the average distance to climb before the  
 338 bypass [22]. In the present work, dislocation climb is assumed to occur for the bypass  
 339 of both, dislocation and MX precipitate obstacles. Therefore, the average waiting time  
 340 of climb for edge dislocation can be expressed as:

$$341 \quad \frac{1}{t_{w,c,i}^s} = R_e \frac{|v_c^s|}{l_i} \quad (21)$$

342 The absolute value of  $v_c^s$  is used here because a dislocation can climb over the  
 343 obstacle in both positive and negative directions.  $l_i$  represents the average climb  
 344 distance to bypass the obstacles.  $R_e$ , denoting the proportion of edge dislocations, is  
 345 introduced since only edge dislocations contributes to the climb process. In BCC  
 346 structures, the nucleation of the double kink structure is frequent. The motion of the  
 347 edge (or screw) dislocations will result in the elongation of the screw (or edge)  
 348 dislocation kinks [46,61]. Since the edge dislocations glide much faster in BCC  
 349 material, the density of edge dislocations is usually limited. In this work,  
 350  $R_e = \rho_{edge} / \rho = 10\%$  is estimated.

351 Arzt et al. [19,20] studied the attractive interaction between the climbing  
 352 dislocation and particles, as a results of which, the edge dislocations may still be  
 353 attached to the hard particles after the climb-over process. An extra detachment  
 354 process is required before it can continue to glide. However, this is not included in the  
 355 proposed model since for the Fe-Cr alloy this process has not been studied in detail.  
 356 Consequently, the climb rate for the precipitate obstacles may be overestimated in this  
 357 work.

### 358 **2.3 Dislocation density law**

359 The dislocation density evolution plays a key role in the present thermal creep  
 360 model. The variance of strain rate for the modified 9Cr-1Mo steel is mainly controlled  
 361 by the evolution of the dislocation density in the subgrain [4]. The dislocation density  
 362 evolution processes considered in this model for  $\dot{\rho}_{cell}^s$  are dislocation generation  
 363 ( $\dot{\rho}_{cell,g}^{s,+}$ ), dynamic recovery due to multiple mechanisms ( $\dot{\rho}_{cell,a}^{s,-}$ ) and trapping at the  
 364 cell walls ( $\dot{\rho}_{cell,trap}^{s,-}$ ):

$$365 \quad \dot{\rho}_{cell}^s = \dot{\rho}_{cell,g}^{s,+} - \dot{\rho}_{cell,a}^{s,-} - \dot{\rho}_{cell,trap}^{s,-} \quad (22)$$

366 The dislocation generation process concerns the expansion of the pinned dislocation  
 367 segments. The generation rate is related to the area swept by the moving dislocations.  
 368 The term  $\dot{\rho}_{cell}^{s,+}$  is determined by a commonly used expression [62–64]:

$$369 \quad \dot{\rho}_{cell,g}^{s,+} = \frac{k_1}{b\lambda^s} |\bar{\gamma}^s| \quad (23)$$

370 The dynamic recovery process involves many mechanisms. The most important ones  
 371 are suggested to be cross-slip and climb [24,65]. The moving dislocation can  
 372 cross-slip and annihilate if it encounters a dislocation with opposite Burger vector. In  
 373 the classic Kocks-Mecking law [65–68], the dynamic recovery term can be written as:

$$374 \quad \dot{\rho}_{cell,a}^{s,-} = f \rho_{cell}^s |\dot{\gamma}| \quad (24)$$

375 here  $f$  is the recovery parameter. It is suggested to be a function of temperature and  
 376 strain rate [65–68]. In many works addressing plastic deformation with high applied  
 377 stress, i.e. [64,68], this parameter is considered as weakly dependent on the strain rate  
 378 (or completely insensitive). Estrin [65] indicated that the strain rate sensitivity of  $f$   
 379 is in fact associated with the dominant mechanism. Compared to cross-slip, the  $f$   
 380 parameter should be more sensitive to strain rate in the climb governed process. Estrin  
 381 [65] also proposed a general expression for  $f$  as:

$$382 \quad f = k_2 \left( \frac{\dot{\epsilon}_0}{\dot{\epsilon}} \right)^{\frac{1}{n_0}} \quad (25)$$

383 where  $\dot{\epsilon}_0$  is a reference strain rate and  $n_0$  is related to the strain rate sensitivity.  
 384 The value of  $n_0$  should be around 3-5 for high temperature cases (climb dominated  
 385 recovery), or higher in low temperature regime where recovery is mainly controlled  
 386 by cross-slip [65]. Using a geometric reasoning, moving dislocation may be  
 387 immobilized after it swept a certain area [22,39,69]. Therefore, the trapping term in  
 388 the present model is given by:

$$389 \quad \dot{\rho}_{cell,trap}^{s,-} = \frac{k_3}{\lambda_{sg}} |\dot{\gamma}| \quad (26)$$

390 where the  $\lambda_{sg}$  represents the sub-grain size. As mentioned in section 2.1,  $\lambda_{sg}$  is  
 391 assumed to be constant throughout the creep test in this work. In Eqs. 23-26,  $k_1$ ,  $k_2$   
 392 and  $k_3$  are material constants.

393 The evolution of the dislocation density in the cell wall is determined through the  
 394 trapping of the moving dislocations and the annihilation process, written as:

$$395 \quad \dot{\rho}_{cw}^s = \dot{\rho}_{cell,trap}^{s,-} - \dot{\rho}_{cw,a}^{s,-} \quad (27)$$

396 Different from the dynamic recovery in Eqs. 24 and 25, the annihilation in the cell  
 397 wall is only controlled by climb since the trapped dislocations cannot glide [27]. Nes  
 398 [24] suggested that the climb-only annihilation rate is proportional to the dislocation  
 399 climb velocity and current dislocation density, and inversely proportional to the  
 400 average dipole separation ( $l_g$ ) as  $\dot{\rho}_{climb}^{s,-} \propto \rho^s |v_c^s| / l_g$ .  $l_g$  scales with  $1/\sqrt{\rho_{cw}^s}$ .  
 401 Therefore:

$$402 \quad \dot{\rho}_{cw,a}^{s,-} = k_c |v_c^s| (\rho_{cw}^s)^{\frac{3}{2}} \quad (28)$$

403  $k_c$  is a material constant and the climb velocity  $v_c^s$  is given in Eq. 20.

## 404 2.4 Brief description of VPSC model

405 The detailed description of VPSC model can be found in Refs. [31,70]. In this  
 406 work, the VPSC framework is used as a platform for calculating the interaction  
 407 between the effective medium representing the macroscopic polycrystal and the  
 408 individual grains. The self-consistent model treats each grain as an inhomogeneous  
 409 visco-plastic inclusion embedded in the “homogeneous effective medium” (HEM).  
 410 Deformation takes place either by enforcing a macroscopic deformation rate or  
 411 imposing a stress for prescribed time increment. The latter case corresponds to creep.  
 412 The total strain rate in one grain is given by the sum of the shear rates of all systems  
 413 (Eq. 1). Its linearized form is written as:

$$414 \quad \dot{\varepsilon}_{ij}^g = M_{ijkl}^g \sigma_{kl} + \dot{\varepsilon}_{ij}^{0,g} \quad (29)$$

415 where  $M_{ijkl}^g$  and  $\dot{\varepsilon}_{ij}^{0,g}$  are the visco-plastic compliance and the back-extrapolated  
 416 rate of grain  $g$ , respectively.  $M_{ijkl}^g$  should be calculated as [35]:

$$417 \quad M_{ijkl}^g = \frac{\partial \dot{\varepsilon}_{ij}^g}{\partial \sigma_{kl}} = \sum_s \frac{\partial \bar{\gamma}}{\partial \bar{\tau}^s} \frac{\partial \bar{\tau}^s}{\partial \sigma_{kl}} m_{ij} = \sum_s \frac{\partial \bar{\gamma}}{\partial \bar{\tau}^s} m_{ij} m_{kl} \quad (30)$$

418 Similar to Eq. 29, the relationship between the strain rate and stress for the aggregate  
 419 is expressed as a linearized form:

$$420 \quad \bar{\varepsilon}_{ij} = \bar{M}_{ijkl} \bar{\sigma}_{kl} + \bar{\varepsilon}_{ij}^0 \quad (31)$$

421 with  $\bar{\varepsilon}_{ij}$ ,  $\bar{\sigma}_{kl}$ ,  $\bar{M}_{ijkl}$ , and  $\bar{\varepsilon}_{ij}^0$  denoting the macroscopic strain rate, stress,  
 422 visco-plastic compliance tensor and back-extrapolated rate, respectively. The  
 423 interaction between the single crystal and the surrounding effective medium in the  
 424 VPSC model is expressed in the interaction law:

$$425 \quad \dot{\varepsilon}_{ij}^g - \bar{\varepsilon}_{ij} = -\tilde{M}_{ijkl} (\sigma_{kl}^g - \bar{\sigma}_{kl}) \quad (32)$$

426 The interaction tensor  $\tilde{M}_{ijkl}$  takes into account the grain shape effect via the Eshelby  
 427 tensor  $S$  as:

$$428 \quad \tilde{M}_{ijkl} = (I - S)_{ijmn}^{-1} S_{mnpq} \bar{M}_{pqkl} \quad (33)$$

## 429 3 Simulation results and discussion

430 The experimental data used to evaluate the proposed model is provided by Basirat  
 431 et al. [14] for the modified Fe-9Cr-1Mo alloy. Prior to the creep tests, this material has

432 been normalized at 1311K (1038°C) for 4h and tempered at 1061K (788°C) for 43min.  
433 The resulting microstructure (initial status for the tests) is consistent with the chosen  
434 paradigm (see section 2.1). The detailed description can be found in Ref [13] from the  
435 same group.

### 436 **3.1 Parameter calibration and simulation conditions**

437 The parameters involved in the simulations are discussed in this section. The  
438 affine interaction in the VPSC framework is used in this work. The average size of  
439 MX precipitates reported in Ref [13] is around 37 nm. The precipitate number density  
440 and trapping parameter are chosen to be  $3 \times 10^{20} \text{ m}^{-3}$  and 1, respectively. This leads to  
441 the mean spacing  $\lambda_{MX}^s = 1/h_{MX} \sqrt{N_{MX} d_{MX}} \approx 300 \text{ nm}$ . This value is in the reasonable range  
442 according to Ref [6]. In the hardening law, the dislocation-dislocation interaction  
443 parameters  $\alpha^{ss'}$  are chosen based on the data in Ref. [71]. The hardening  
444 superposition factor  $m$  is set to 2 as given in Refs [42,49,50]. In the Kocks type law  
445 (Eqs. 13 and 14), the parameter  $\Delta G_{0,\rho}$ ,  $\Delta G_{0,MX}$ ,  $\nu_{G,MX}$ ,  $p$  and  $q$  are obtained by  
446 back fitting the experimental data within reasonable ranges ( $\nu_{G,i} \approx 10^{10} - 10^{11} \text{ s}^{-1}$  [22];  
447  $0 < p \leq 1$  and  $1 \leq p < 2$  [48]). The lattice friction stress  $\tau_0^s$  is in general a function  
448 of temperature. However, according to Gilbert et al. [72], in Fe this stress decreases  
449 with increasing temperature and vanishes at 700K (427°C). Therefore, for the  
450 temperature interval studied in this work, which is above 873K (600°C),  $\tau_0^s$  is set to  
451 be 0.

452 In this work, the initial values of  $\rho_{cell}^s$  and  $\rho_{cw}^s$  for each system are chosen to be  
453  $4 \cdot 10^{12} \text{ m}^{-2}$  and  $1 \cdot 10^{13} \text{ m}^{-2}$ , respectively. Hence the densities in the cell and in the cell  
454 wall start at  $9.6 \cdot 10^{13} \text{ m}^{-2}$  and  $2.4 \cdot 10^{14} \text{ m}^{-2}$ , respectively. In this way, the total  
455 dislocation density is of the order  $10^{14} \text{ m}^{-2}$  and the one in the cell wall is higher than  
456 that in the cell, which agrees with the experimental observations [14,73–75]. The  
457 evolution related parameters  $k_1$ ,  $k_2$ ,  $k_3$  and  $k_c$  are calibrated according to the  
458 experimental data. The strain rate sensitivity parameter  $n_0$  in the dislocation dynamic  
459 recovery term depends on the annihilation mechanisms [65]. Its value is chosen to be  
460 3.5 in this work and the rationality will be discussed in the following sections.

461 The vacancy diffusivity and the equilibrium concentration of vacancies are  
462 important parameters affecting the climb process. They are determined using  
463 molecular dynamics simulation data reported by Mendelev and Mishin [76] for BCC  
464 Fe. The diffusivity is calculated by:

465  $D_v = D_v^0 \exp(-E_m^v/kT)$  (34)

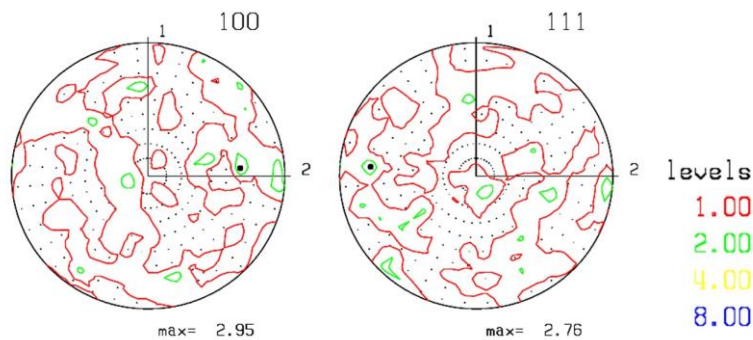
466 where the vacancy migration energy  $E_m^v$  is 0.6 eV and the diffusion constant  $D_v^0$  is  
 467  $7.87 \times 10^{-7} \text{ m}^2/\text{s}$ . The vacancy formation energy and entropy are given as function of  
 468 temperature:

469  $E_f^v = g_0 - g_2 T^2 - 2g_3 T^3$   
 $S_f^v = -g_1 - 2g_2 T - 3g_3 T^2$  (35)

470 The  $g_x$  coefficients and the other parameters involved in the calculation of  
 471 dislocation waiting time are listed in Table 1.

472 Since the cladding material exhibits a weak texture, an initial texture consisting of  
 473 100 random orientations (Fig. 4) is utilized as input. The  $\{110\}\langle 111 \rangle$  and  $\{112\}\langle 111 \rangle$   
 474 slip modes are assumed to be active in BCC Fe-Cr-Mo steel. The tensile creep tests  
 475 are simulated under stress-controlled boundary conditions: stress along axis 3 ( $\Sigma_{33}$ ) is  
 476 imposed and the rest of the stress components  $\Sigma_{ij}$  are enforced to be zero.

477 The experimental data used to adjust and benchmark the proposed model is taken  
 478 from available literature [14]. The same temperatures and creep stresses will be  
 479 applied in the simulations. The results will be presented in section 3.3. Notice that  
 480 only the primary creep stage and steady-state stage of thermal creep will be simulated.  
 481 The third stage, where the creep rate shows an evident increase, is usually attributed  
 482 to void nucleation and crack formation [41,77] and is out of the scope of the present  
 483 modeling framework.



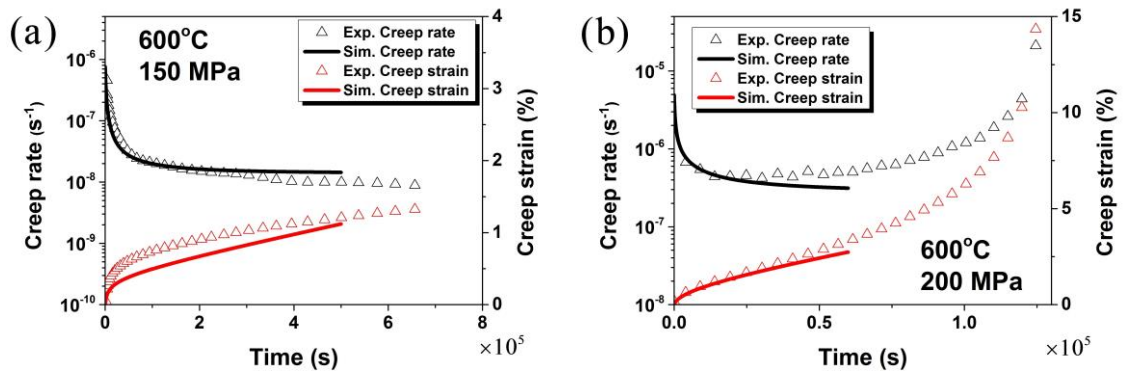
484  
 485 Fig. 3. Pole figures for the initial random texture with 100 grains.

### 486 3.2 Simulation results

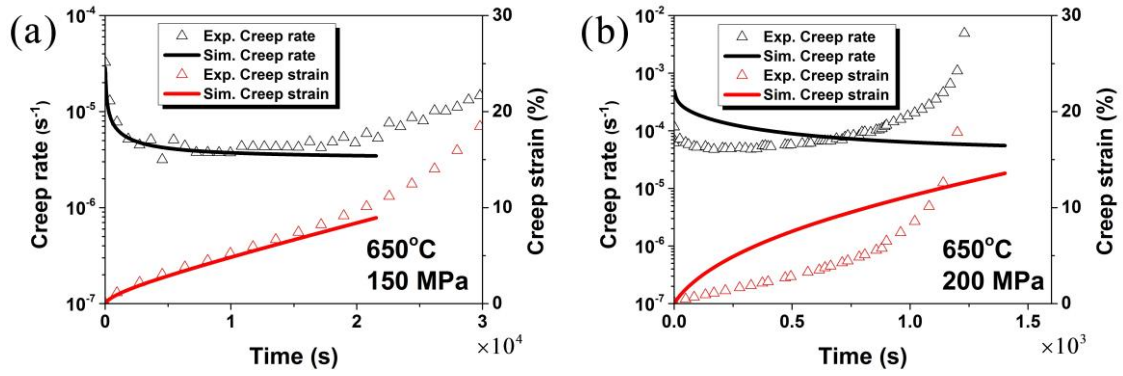
487 The creep rate and the creep strain in Basirat et al. [14] are measured under the

488 following conditions: 873K (600°C) with 150 and 200 MPa; 923K (650°C) with 150  
 489 and 200 MPa; 973K (700°C) with 80, 100, 150 and 200 MPa. Figs. 4-7 show the  
 490 comparison of the predicted results with experiments as a function of stress and  
 491 temperature. The most obvious feature in these experiments is the strong dependence  
 492 of the creep rate with applied stress. Differences of 50 MPa or even 20 MPa impact  
 493 strongly on the creep rates observed. Despite such demanding experimental conditions,  
 494 reasonable agreement is obtained for both. Notice that the experimental data in Basirat  
 495 et al. show an obvious power-law regime behavior [13,14]. Therefore, the diffusion  
 496 creep, which is excluded from this model, will not evidently affect the prediction in  
 497 this work.

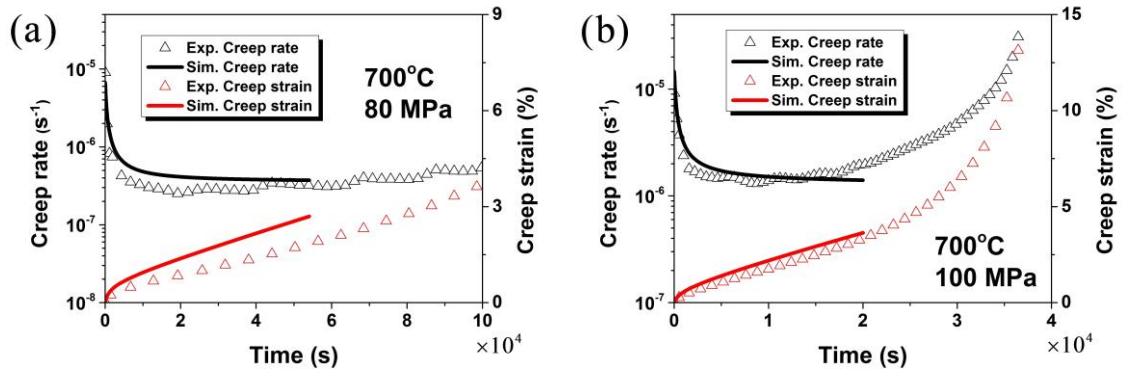
498 It can be seen that the simulation results capture the evolution for both the creep  
 499 rate and creep strain curves over a wide range of orders of magnitudes. Still, some  
 500 discrepancies are apparent in Figs. 4-7, the possible causes for which are discussed in  
 501 what follows. First, a random texture is used in this work due to the lack of  
 502 experimental texture data. Another possible source of error could be the initial  
 503 dislocation densities used, which are the same for all tests in this work. However, they  
 504 are likely to be different depending on the temperature, which will induce some  
 505 annealing. The parameters controlling the waiting time of the thermal-activated glide  
 506 and climb, could also affect the predicted results. These parameters can be better  
 507 calibrated by using the data from more systematic experiments or low scale  
 508 dislocation dynamic simulations.



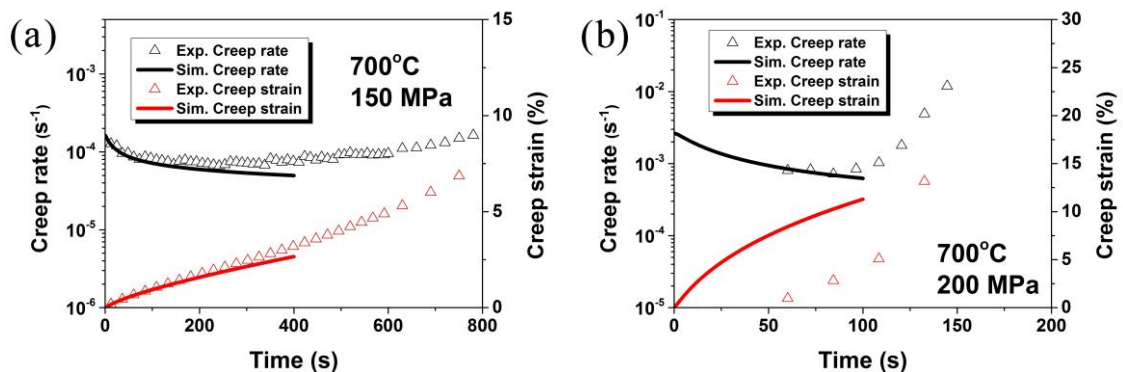
509 Fig. 4. Predicted creep rate and creep strain for Fe-Cr-Mo steel at 873K (600°C) with  
 510 applied stress of 150 (a) and 200 MPa (b). Experimental data from Ref. [14].



511 Fig. 5. Predicted creep rate and creep strain for Fe-Cr-Mo steel at 923K (650°C) with  
 512 applied stress of 150 (a) and 200 MPa (b). Experimental data from Ref. [14].



513 Fig. 6. Predicted creep rate and creep strain for Fe-Cr-Mo steel at 973K (700°C) with  
 514 applied stress of 80 (a) and 100 MPa (b). Experimental data from Ref. [14].



515 Fig. 7. Predicted creep rate and creep strain for Fe-Cr-Mo steel at 973K (700°C) with  
 516 applied stress of 150 (a) and 200 MPa (a). Experimental data from Ref. [14].

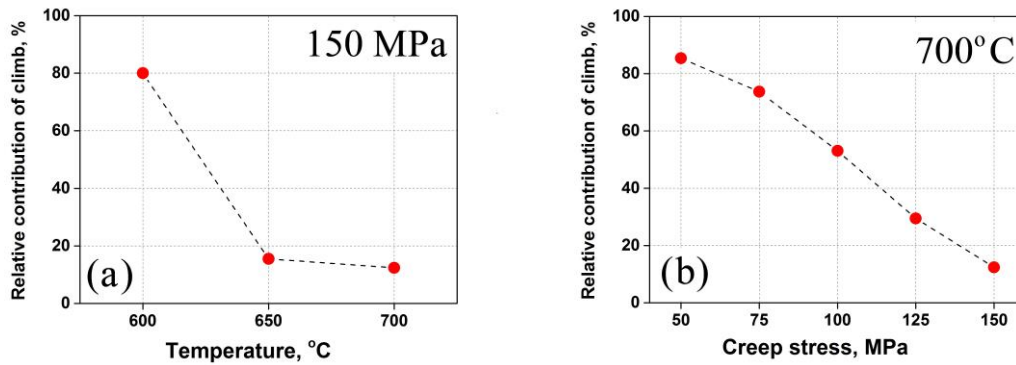
### 517 3.3 Relative contribution of glide and climb mechanisms

518 The proposed modeling framework is able to consider the contribution of both the  
 519 thermally-activated glide and the dislocation climb mechanisms in the deformation



520 process. In order to study their relative activities, we define  $P_c = 1 - \varepsilon_{w/o}^i / \varepsilon_w^i$  to  
 521 describe the percentage of the climb contribution.  $\varepsilon_w^i$  and  $\varepsilon_{w/o}^i$  denote the creep rates  
 522 at the initial step of the simulations with and without considering the climb mechanism  
 523 (using the parameters of Fe-Cr-Mo steel given in section 3.1).

524 Fig. 8 exhibits the predicted relative contribution of climb under various  
 525 temperature and stress. As shown in Fig. 8a, the contribution of climb is relatively  
 526 larger at lower temperature. In this model, the climb process is controlled by the  
 527 temperature-dependent equilibrium vacancy concentration, vacancy diffusivity and the  
 528 chemical force (see Appendix). Thermally-activated glide is also strongly dependent  
 529 on temperature. The results in Fig. 8a indicate that the thermally-activated glide is  
 530 relatively more sensitive to temperature than climb. Fig. 8b demonstrates that the  
 531 relative activity of climb is inversely proportional to the creep stress. It can be  
 532 explained as that the activity of thermally-activated glide shows an exponential growth  
 533 with the stress (Eq.13). On the other hand, the value of  $f_c^s \Omega / kTb$  in Eqs. 19 and 20 is  
 534 low (close to zero). This mathematically leads to a relatively more linear relationship  
 535 between the climb velocity and the applied stress [54].

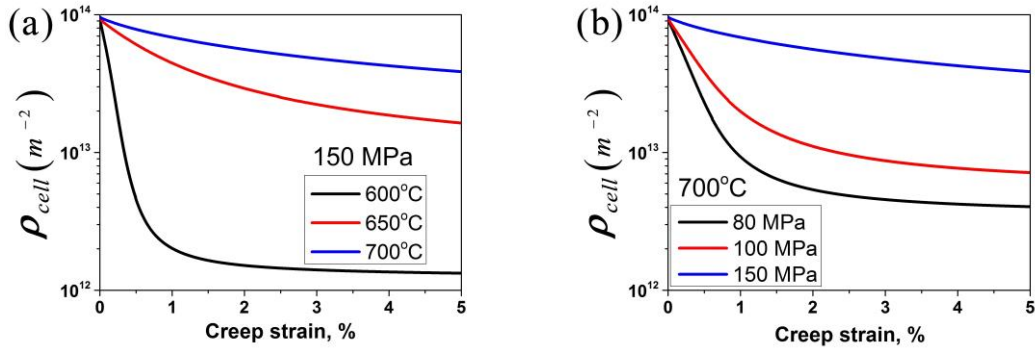


536 Fig. 8. Relative contribution of dislocation climb mechanism as a function of (a)  
 537 temperature and (b) creep stress.

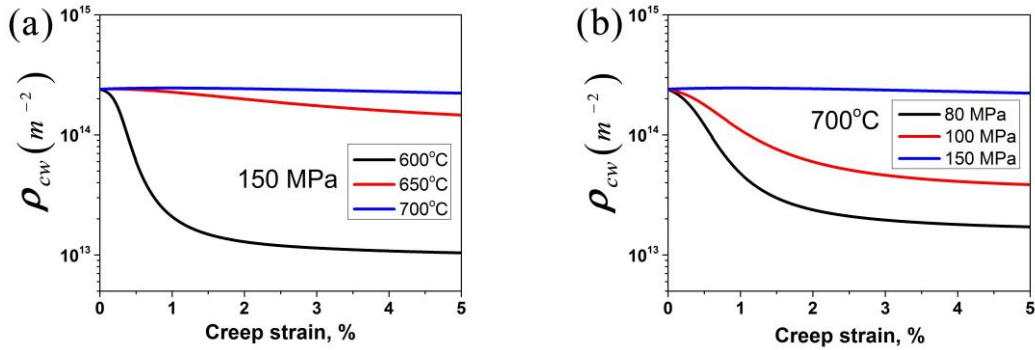
### 538 3.4 Dislocation density evolution

539 The predicted dislocation density evolutions in the subgrain are presented in Fig.  
 540 9. The results are compared at various loading condition. It shows that  $\rho_{cell}$  tends to  
 541 decrease more for lower temperature and/or stress. On the other hand, the evolution of  
 542  $\rho_{cw}$ , given in Fig. 10, shows the same tendency. Notice that the subgrain size, which is  
 543 considered constant in this work, is actually dependent on  $\rho_{cw}$ . It has been reported

544 that the saturation subgrain size, which scales with  $1/\sqrt{\rho_{cw}}$ , is inversely proportional  
 545 to the applied stress [6]. This is in agreement with the present simulations.

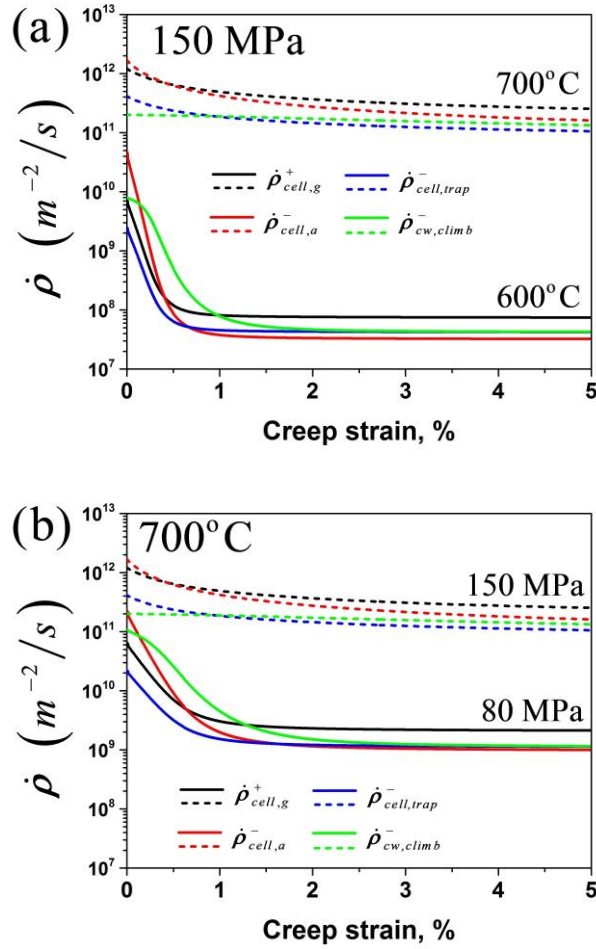


546 Fig. 9. Predicted evolution of dislocation density within subgrains under different  
 547 temperatures (a) and stresses (b)



548 Fig. 10. Predicted evolutions of dislocation density in the cell walls under different  
 549 temperatures (a) and stresses (b)

551 In Fig. 11 the roles of each dislocation density evolution term ( $\dot{\rho}_{cell,g}^{s,+}$ ,  $\dot{\rho}_{cell,a}^{s,-}$ ,  
 552  $\dot{\rho}_{cell,trap}^{s,-}$  and  $\dot{\rho}_{cw,climb}^{s,-}$ ) are analyzed. By summing the components from individual slip  
 553 systems and then averaging these values across all grains, the macroscopic  $\dot{\rho}_{cell,g}^{s,+}$ ,  
 554  $\dot{\rho}_{cell,a}^{s,-}$ ,  $\dot{\rho}_{cell,trap}^{s,-}$  and  $\dot{\rho}_{cw,climb}^{s,-}$  are calculated for the polycrystal. For lower stress and  
 555 temperature cases, we can see that the value for  $\dot{\rho}_{cell,a}^{s,-}$  is relatively high at the  
 556 beginning of the tests. This indicates that the dynamic recovery process dominates the  
 557 drop of  $\rho_{cell}$  (and hence the creep rate) in the primary creep regime. This term later  
 558 becomes very weak in the steady state due to the large decrease of  $\rho_{cell}$  and creep  
 559 rate.

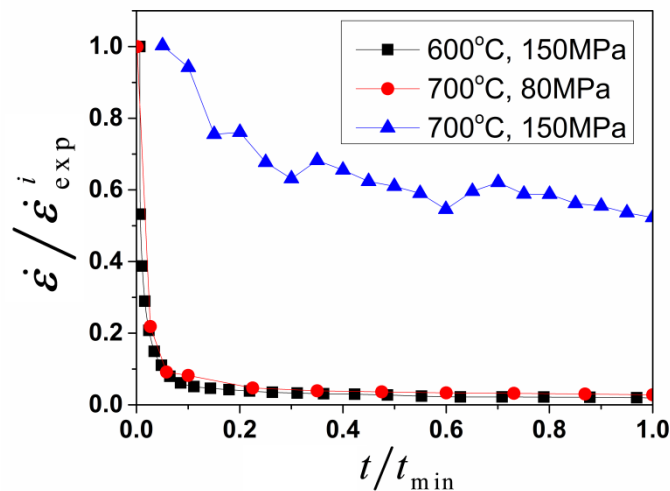


560 Fig.11. Contribution for the dislocation density evolution related mechanisms for  
 561 different temperatures (a) and stresses (b).

562 The experimental data used in this work [14] show an important dependence of  
 563 the creep rate evolution with stress and temperature. In Fig. 12, some of the  
 564 experimental creep rate curves are presented for different stresses and temperatures.  
 565 The strain rate data are normalized by the initial strain rate in the experimental data  
 566  $\dot{\epsilon}_{exp}$ , whereas the time is normalized by  $t_{min}$ , the time where the experimental  
 567 minimum creep rate appears. Although the initial creep rate is not accurately indicated  
 568 by experiments, we can see that  $\dot{\epsilon}$  tends to decrease by a larger fraction when a  
 569 lower stress or temperature is applied. As presented in Fig. 13a, such behavior is  
 570 reproduced by the proposed model. Here the predicted strain curves (using the  
 571 parameters listed in Table 1) are normalized by the strain rate at the first step of the  
 572 simulations.

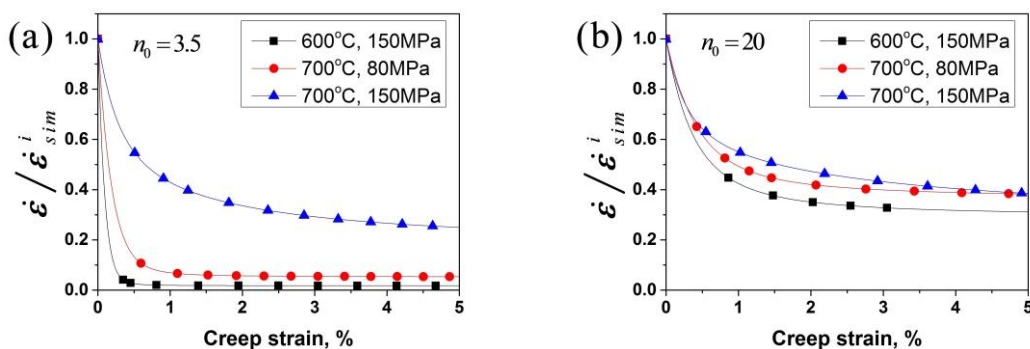
573 In the proposed model, the dynamic recovery process plays a key role in the  
 574 evolution of dislocation population in the subgrain, which is responsible for capturing  
 575 the tendency in experiments. Eq. 25 shows that dynamic recovery is a function of

576 strain rate with sensitivity is governed by  $n_0$ . According to Estrin [65],  $n_0$  should be  
577 a constant (around 3-5) for high temperature cases where climb is the dominant  
578 mechanism in dynamic recovery. For low temperature cases (cross-slip controlled  
579 process), its value should be much higher (of order 20 as in Ref. [78]). The boundary  
580 between the two temperature regimes is not clear and is supposed to vary depending  
581 on the material. In this work,  $n_0 = 3.5$  is used in the simulations. Otherwise, the strain  
582 rate evolution in cannot be captured accordingly with experimental data. In Fig. 13b,  
583 the simulation is carried out using  $n_0 = 20$  and the parameter  $k_2$  is set to 600 to fit  
584 the reference experimental results (973K (700°C) and 150 MPa). It shows that the  
585 predicted strain rate does not vary evidently under different loading conditions. This  
586 result implies dislocation climb is the dominant mechanisms for dynamic recovery  
587 process in the conducted creep tests.



588

589 Fig. 12. Experimental creep rate evolution under different stresses and temperatures.  
590 Creep rate and time normalized by the initial creep rate and the time that the minimum  
591 creep rate presents respectively. Experimental data from Ref. [14].



592 Fig. 13. Predicted creep rate evolution under different stresses and temperatures using

593 (a)  $n_0 = 3.5$  and (b)  $n_0 = 20$ . Creep rate normalized by the initial creep rate.

594 As mentioned in section 2.1, the growth of MX and  $M_{23}C_6$  precipitates is  
595 neglected in this model, as well as the precipitation of Laves-phase and Z-phase. We  
596 believe this should not affect the results in the present simulations. The experimental  
597 results in Basirat et al. [14] correspond to short term creep tests with a total creep time  
598 less than 200h. A rough estimate from the data in Ref. [7] indicates that the size of  
599 MX and  $M_{23}C_6$  precipitates will grow less than 0.1% within this time range. Moreover,  
600 the study of Hayakawa et al. [4] shows that the dislocation mobility in modified  
601 9Cr-1Mo steel is not significantly changed during creep tests up to around 7% creep  
602 strain. This proves indirectly that the microstructure of this material is relatively stable  
603 for short-term tests.

604

## 605 **4 Conclusions and perspectives**

606 In this work, a crystallographic thermal creep model is proposed for Fe-Cr alloy.  
607 The thermal-activated glide and climb mechanisms are coupled in the formulation to  
608 determine the mean dislocation waiting time at different types of the obstacle (other  
609 dislocations and MX precipitates). This model, embedded in the VPSC framework,  
610 captures well the thermal creep behavior for modified 9Cr-1Mo steel under various  
611 stresses and temperatures. The relative contribution of thermally-activated glide and  
612 climb mechanisms is evaluated for different creep conditions. The results show that  
613 thermally-activated glide is strongly suppressed for creep at lower temperature, but  
614 makes a relatively higher contribution on the dislocation mobility in high-stress  
615 regime.

616 The dislocation density evolution law, considering multiple mechanisms in the  
617 annihilation process, is also essential to predict correctly the creep behavior for the  
618 initial and steady-state stages. The strain rate sensitive dynamic recovery is the  
619 dominant factor to capture the strain rate variance under various loading conditions.  
620 The dislocation recovery is a sophisticated phenomenon. The physics process is not  
621 completely known. The simulation data in this work imply that dislocation climb could  
622 be the governing mechanism for the dynamic recovery in modified 9Cr-1Mo steel  
623 (within the corresponding stress and temperature intervals). However, more studies are  
624 necessary to unravel its specifics in future.

625

## 626 **Acknowledgment**

627 This work was funded by the US Department of Energy's Nuclear Energy Advanced  
628 Modeling and Simulation (NEAMS). Special thanks go to Prof. G.P. Potirniche for  
629 providing us with the detailed experimental data.

630

631

632 **Appendix**

633 Previous studies [18,46,52–54] show the climb velocity can be expressed as:

$$634 \quad v_c^s = \frac{I_v^s \Omega}{b} \quad (\text{A-1})$$

635 To calculate the vacancy current  $I_v^s$ , one needs to analyze the stress and vacancy  
 636 concentration status around the climbing edge dislocation. A cylindrical control  
 637 volume around the dislocation line with the radius  $r$  is defined. The zone with  
 638  $r \leq r_d$  is considered as the dislocation core region. Therefore the chemical force  
 639 (Osmotic force) applied on the unit length of edge dislocation segment can be  
 640 obtained as [46,79]:

$$641 \quad f_{os}^s = -\frac{kTb}{\Omega} \ln\left(\frac{C_v^s(r_d)}{C_v^0}\right) \quad (\text{A-2})$$

642 where  $C_v^s(r_d)$  represents the vacancy concentration at  $r = r_d$ .  $C_v^0$  is the equilibrium  
 643 vacancy concentration at a given temperature.

644 Meanwhile, climb is also affected by the climb component of Peach-Koehler force.  
 645 The full Peach-Koehler force is defined as  $\mathbf{f} = (\boldsymbol{\sigma} \cdot \mathbf{b}^s) \times \mathbf{t}^s$  where  $\mathbf{t}^s$  is the  
 646 normalized tangent to the dislocation line [56,57]. The climb component of  $\mathbf{f}$  for  
 647 the edge dislocation can be expressed as [58–60]:

$$648 \quad f_c^s = \mathbf{f}^s \cdot \mathbf{n}^s = [(\boldsymbol{\sigma} \cdot \mathbf{b}^s) \times \mathbf{t}^s] \cdot \mathbf{n}^s = -|\mathbf{b}^s| \boldsymbol{\sigma} : (\mathbf{b}^s \otimes \mathbf{b}^s) \quad (\text{A-3})$$

649 When the dislocation is locally in equilibrium state, the total force  $f^s = f_{os}^s + f_c^s$   
 650 should be equal to 0. Therefore we get from Eqs. A-2 and A-3:

$$651 \quad C_v^s(r_d) = C_{v,eq}^s = C_v^0 \exp\left(\frac{-f_c^s \Omega}{kTb}\right) \quad (\text{A-4})$$

652 Notice that the vacancy concentration in the material matrix is assumed to be equal to  
 653 the equilibrium concentration,  $C_v(r \geq r_\infty) = C_v^\infty = C_v^0$ , where  $r_\infty$  denotes the radius of  
 654 the outer boundary for the control volume. Therefore a vacancy concentration  
 655 gradient along the radius appears in the control volume which leads to a diffusive  
 656 flow of vacancies. The dislocation needs to absorb or emit vacancies (climb) to retain  
 657 the local equilibrium status.

658 At steady-state the divergence of vacancy diffusion flux  $J$  is null in the absence of  
 659 defect creation. The associated Laplace equation in the cylindrical coordinate system  
 660 is:

$$661 \quad \nabla^2 C_v^s = \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial C_v^s}{\partial r} = 0 \quad (\text{A-5})$$

662 with the inner and outer boundary conditions:

$$663 \quad \begin{aligned} C_v^s(r=r_\infty) &= C_v^\infty = C_v^0 \\ C_v^s(r=r_d) &= C_{v,eq}^s \end{aligned} \quad (\text{A-6})$$

664 By solving Eq. A-5, we obtain:

$$665 \quad C_v^s(r) = C_{v,eq}^s + (C_v^\infty - C_{v,eq}^s) \frac{\ln(r/r_\infty)}{\ln(r_\infty/r_d)} \quad (\text{A-7})$$

666 Therefore, the net current absorbed or emitted by unit length of dislocation segment is  
667 given by:

$$668 \quad I_v^s = 2\pi r \cdot J = 2\pi r \frac{D_v}{\Omega} \frac{\partial C_v^s(r)}{\partial r} = \frac{2\pi D_v \left[ C_v^\infty - C_v^0 \exp\left(\frac{-f_c^s \Omega}{kTb}\right) \right]}{\Omega \ln(r_\infty/r_d)} \quad (\text{A-8})$$

669 where  $D_v$  is the vacancy diffusivity. Then the climb velocity can be expressed as:

$$670 \quad v_c^s = \frac{I_v^s \Omega}{b} = \frac{2\pi D_v \left[ C_v^\infty - C_v^0 \exp\left(\frac{-f_c^s \Omega}{kTb}\right) \right]}{b \ln(r_\infty/r_d)} \quad (\text{A-9})$$

671

## 672 **References**

- 673 1. F. Abe, *Sci. Technol. Adv. Mater.* **9**, 13002 (2008).
- 674 2. E. Cerri, E. Evangelista, S. Spigarelli, and P. Bianchi, *Mater. Sci. Eng. A* **245**, 285  
675 (1998).
- 676 3. H. K. Danielsen, *Mater. Sci. Technol.* **836**, 1743284715Y.000 (2015).
- 677 4. H. Hayakawa, S. Nakashima, J. Kusumoto, A. Kanaya, and H. Nakashima, *Int. J.*  
678 *Press. Vessel. Pip.* **86**, 556 (2009).
- 679 5. S. Yamasaki, *Modelling Precipitation of Carbides in Martensitic Steels*, 2009.
- 680 6. K. Maruyama, K. Sawada, and J. Koike, *ISIJ Int.* **41**, 641 (2001).
- 681 7. T. Nakajima, S. Spigarelli, E. Evangelista, and T. Endo, *Mater. Trans.* **44**, 1802  
682 (2003).
- 683 8. J. Hald, *Int. J. Press. Vessel. Pip.* **85**, 30 (2008).
- 684 9. Y. Yamamoto, B. A. Pint, K. A. Terrani, K. G. Field, Y. Yang, and L. L. Snead, *J.*  
685 *Nucl. Mater.* **467**, 703 (2015).
- 686 10. K. G. Field, M. N. Gussev, Y. Yamamoto, and L. L. Snead, *J. Nucl. Mater.* **454**,  
687 352 (2014).

- 688 11. K. G. Field, X. Hu, K. C. Littrell, Y. Yamamoto, and L. L. Snead, *J. Nucl. Mater.*  
689 **465**, 746 (2015).
- 690 12. T. Shrestha, M. Basirat, I. Charit, G. P. Potirniche, and K. K. Rink, *Mater. Sci.*  
691 *Eng. A* **565**, 382 (2013).
- 692 13. T. Shrestha, M. Basirat, I. Charit, G. P. Potirniche, K. K. Rink, and U. Sahaym, *J.*  
693 *Nucl. Mater.* **423**, 110 (2012).
- 694 14. M. Basirat, T. Shrestha, G. P. Potirniche, I. Charit, and K. Rink, *Int. J. Plast.* **37**,  
695 95 (2012).
- 696 15. M. Tamura, H. Sakasegawa, A. Kohyama, H. Esaka, and K. Shinozuka, *J. Nucl.*  
697 *Mater.* **321**, 288 (2003).
- 698 16. M. Taneike, F. Abe, and K. Sawada, *Nature* **424**, 294 (2003).
- 699 17. S. Spigarelli, E. Cerri, P. Bianchi, and E. Evangelista, (2016).
- 700 18. G. S. Was, *Fundamentals of Radiation Materials Science: Metals and Alloys*  
701 (Springer Science & Business Media, 2007).
- 702 19. E. Arzt and J. Rosler, *Acta Metall.* **36**, 1053 (1988).
- 703 20. E. Arzt and D. S. Wilkinson, *Acta Metall.* **34**, 1893 (1986).
- 704 21. J. Roesler and E. Arzt, *Acta Metall.* **36**, 1043 (1988).
- 705 22. A. Patra and D. L. McDowell, *Philos. Mag.* **92**, 861 (2012).
- 706 23. Y. Qin, G. Götz, and W. Blum, *Mater. Sci. Eng. A* **341**, 211 (2003).
- 707 24. E. Nes, *Prog. Mater. Sci.* **41**, 129 (1997).
- 708 25. Y. Estrin and H. Mecking, *Acta Metall.* **32**, 57 (1984).
- 709 26. G. Gottstein and A. S. Argon, *Acta Metall.* **35**, 1261 (1987).
- 710 27. F. Roters, D. Raabe, and G. Gottstein, *Acta Mater.* **48**, 4181 (2000).
- 711 28. Y. Xiang and D. J. Srolovitz, *Philos. Mag.* **86**, 3937 (2006).
- 712 29. R. Oruganti, *Acta Mater.* **60**, 1695 (2012).
- 713 30. R. A. Lebensohn and C. N. Tomé, *Acta Metall. Mater.* **41**, 2611 (1993).
- 714 31. R. A. Lebensohn, C. N. Tomé, and P. P. Castañeda, *Philos. Mag.* **87**, 4287  
715 (2007).
- 716 32. B. Fournier, M. Sauzay, and A. Pineau, *Int. J. Plast.* **27**, 1803 (2011).
- 717 33. L. S. Tóth, A. Molinari, and Y. Estrin, *J. Eng. Mater. Technol.* **124**, 71 (2002).
- 718 34. Y. Estrin, L. S. Tóth, A. Molinari, and Y. Bréchet, *Acta Mater.* **46**, 5509 (1998).
- 719 35. H. Wang, B. Clausen, L. Capolungo, I. J. Beyerlein, J. Wang, and C. N. Tomé, *Int.*



720 J. Plast. **79**, 275 (2016).

721 36. H. Wang, L. Capolungo, B. Clausen, and C. N. Tomé, Int. J. Plast. (2016).

722 37. J. T. Lloyd, J. D. Clayton, R. A. Austin, and D. L. McDowell, J. Mech. Phys.  
723 Solids **69**, 14 (2014).

724 38. R. J. Clifton, (1971).

725 39. R. A. Austin and D. L. McDowell, Int. J. Plast. **27**, 1 (2011).

726 40. P. Franciosi and A. Zaoui, Acta Metall. **30**, 1627 (1982).

727 41. N. Bertin, C. N. Tomé, I. J. Beyerlein, M. R. Barnett, and L. Capolungo, Int. J.  
728 Plast. **62**, 72 (2014).

729 42. C. Sobie, N. Bertin, and L. Capolungo, Metall. Mater. Trans. A Phys. Metall.  
730 Mater. Sci. **46**, 3761 (2015).

731 43. G. E. Lucas, J. Nucl. Mater. **206**, 287 (1993).

732 44. C. Deo, C. N. Tomé, R. Lebensohn, and S. Maloy, J. Nucl. Mater. **377**, 136  
733 (2008).

734 45. J. Friedel, in (Wiley, New York, 1963), p. 605.

735 46. J. P. Hirth and J. Lothe, J. Appl. Mech. **50**, 476 (1983).

736 47. V. Gaffard, Experimental Study and Modelling of High Temperature Creep Flow  
737 and Damage Behaviour of 9Cr1Mo-NbV Steel Weldments, 2004.

738 48. U. F. Kocks, A. S. Argon, and M. F. Ashby, Prog. Mater. Sci. **19**, 171 (1975).

739 49. U. Lagerpusch, V. Mohles, D. Baither, B. Anczykowski, and E. Nembach, Acta  
740 Mater. **48**, 3647 (2000).

741 50. Y. Dong, T. Nogaret, and W. A. Curtin, Metall. Mater. Trans. A Phys. Metall.  
742 Mater. Sci. **41**, 1954 (2010).

743 51. A. V. Granato, K. Lücke, J. Schlipf, and L. J. Teutonico, J. Appl. Phys. **35**, 2732  
744 (1964).

745 52. M. G. D. Geers, M. Cottura, B. Appolaire, E. P. Busso, S. Forest, and A. Villani, J.  
746 Mech. Phys. Solids **70**, 136 (2014).

747 53. B. Bakó, E. Clouet, L. M. Dupuy, and M. Blétry, Philos. Mag. **91**, 3173 (2011).

748 54. Y. Gu, Y. Xiang, S. S. Quek, and D. J. Srolovitz, J. Mech. Phys. Solids **83**, 319  
749 (2014).

750 55. D. Mordehai, E. Clouet, M. Fivel, and M. Verdier, Philos. Mag. **88**, 899 (2008).

751 56. J. Weertman, Philos. Mag. **11**, 1217 (1965).

752 57. J. Weertman and J. R. Weertman, *Elementary Dislocation Theory* (Oxford

753 University Press, Oxford, 1992).

754 58. R. A. Lebensohn, C. S. Hartley, C. N. Tomé, and O. Castelnau, *Philos. Mag.* **90**,  
755 567 (2010).

756 59. R. A. Lebensohn, R. A. Holt, A. Caro, A. Alankar, and C. N. Tomé, *Comptes*  
757 *Rendus - Mec.* **340**, 289 (2012).

758 60. C. S. Hartley, *Philos. Mag.* **83**, 3783 (2003).

759 61. J. Chang, W. Cai, V. V Bulatov, and S. Yip, *Mater. Sci. Eng. A* **309–310**, 160  
760 (2001).

761 62. W. Wen, M. Borodachenkova, C. N. Tomé, G. Vincze, E. F. Rauch, F. Barlat, and  
762 J. J. Grácio, *Acta Mater.* **111**, 305 (2016).

763 63. W. Wen, M. Borodachenkova, C. N. Tomé, G. Vincze, E. F. Rauch, F. Barlat, and  
764 J. J. Grácio, *Int. J. Plast.* **73**, 171 (2015).

765 64. K. Kitayama, C. N. Tomé, E. F. Rauch, J. J. Gracio, and F. Barlat, *Int. J. Plast.* **46**,  
766 54 (2013).

767 65. Y. Estrin, *J. Mater. Process. Technol.* **80–81**, 33 (1998).

768 66. U. F. Kocks and H. Mecking, *Prog. Mater. Sci.* **48**, 171 (2003).

769 67. H. Mecking and U. F. Kocks, *Acta Metall.* **29**, 1865 (1981).

770 68. I. J. Beyerlein and C. N. Tomé, *Int. J. Plast.* **24**, 867 (2008).

771 69. U. F. Kocks, *Philos. Mag.* **13**, 541 (1966).

772 70. H. Wang, B. Raeisinia, P. D. Wu, S. R. Agnew, and C. N. Tomé, *Int. J. Solids*  
773 *Struct.* **47**, 2905 (2010).

774 71. S. Queyreau, G. Monnet, and B. Devincre, *Int. J. Plast.* **25**, 361 (2009).

775 72. M. R. Gilbert, P. Schuck, B. Sadigh, and J. Marian, *Phys. Rev. Lett.* **111**, 1  
776 (2013).

777 73. C. G. Panait, A. Zielińska-Lipiec, T. Koziel, A. Czyrska-Filemonowicz, A.-F.  
778 Gourgues-Lorenzon, and W. Bendick, *Mater. Sci. Eng. A* **527**, 4062 (2010).

779 74. S. Hollner, B. Fournier, J. Le Pendu, T. Cozzika, I. Tournié, J. C. Brachet, and A.  
780 Pineau, *J. Nucl. Mater.* **405**, 101 (2010).

781 75. S. D. Yadav, S. Kalácska, M. Dománková, D. C. Yubero, R. Resel, I. Groma, C.  
782 Beal, B. Sonderegger, C. Sommitsch, and C. Poletti, *Mater. Charact.* **115**, 23 (2016).

783 76. M. I. Mendeleev and Y. Mishin, *Phys. Rev. B - Condens. Matter Mater. Phys.* **80**, 1  
784 (2009).

785 77. V. Gaffard, A. F. Gourgues-Lorenzon, and J. Besson, *Nucl. Eng. Des.* **235**, 2547  
786 (2005).

- 787 78. J. Li and A. K. Soh, *Int. J. Plast.* **39**, 88 (2012).
- 788 79. H. Wiedersich and K. Herschbach, *Scr. Metall.* **6**, 453 (1972).
- 789

790 **Figure captions:**

791 Fig. 1. Schematic view of the microstructure for heat treated high Cr steels.

792 Fig. 2. Schematic view of the obstacle-bypass mechanisms for moving dislocations.

793 Fig. 3. Pole figures for the initial random texture with 100 grains.

794 Fig. 4. Predicted creep rate and creep strain for Fe-Cr-Mo steel at 873K (600°C) with  
795 applied stress of 150 (a) and 200 MPa (b). Experimental data from Ref. [14].

796 Fig. 5. Predicted creep rate and creep strain for Fe-Cr-Mo steel at 923K (650°C) with  
797 applied stress of 150 (a) and 200 MPa (b). Experimental data from Ref. [14].

798 Fig. 6. Predicted creep rate and creep strain for Fe-Cr-Mo steel at 973K (700°C) with  
799 applied stress of 80 (a) and 100 MPa (b). Experimental data from Ref. [14].

800 Fig. 7. Predicted creep rate and creep strain for Fe-Cr-Mo steel at 973K (700°C) with  
801 applied stress of 150 (a) and 200 MPa (b). Experimental data from Ref. [14].

802 Fig. 8. Relative contribution of dislocation climb mechanism as a function of (a)  
803 temperature and (b) creep stress.

804 Fig. 9. Predicted evolution of dislocation density within subgrains under different  
805 temperatures (a) and stresses (b)

806 Fig. 10. Predicted evolutions of dislocation density in the cell walls under different  
807 temperatures (a) and stresses (b)

808 Fig.11. Contribution for the dislocation density evolution related mechanisms for  
809 different temperatures (a) and stresses (b).

810 Fig. 12. Experimental creep rate evolution under different stresses and temperatures.  
811 Creep rate and time normalized by the initial creep rate and the time that the minimum  
812 creep rate presents respectively. Experimental data from Ref. [14].

813 Fig. 13. Predicted creep rate evolution under different stresses and temperatures using  
814 (a)  $n_0 = 3.5$  and (b)  $n_0 = 20$ . Creep rate normalized by the initial creep rate.

815 **Tables:**

816 Table 1. Parameters used for the Fe-Cr-Mo alloy in this work

817

818

819

Table 1. Parameters used for the Fe-Cr-Mo alloy in this work

Parameters	Fe-Cr-Mo	
$\rho_0$ (mass density)	8000 Kg/m <sup>3</sup>	
$b$ (magnitude of Burgers vector)	$2.48 \cdot 10^{-10}$ m	
$\mu$ (shear modulus)	$103572 \text{ MPa} - T \cdot 48 \text{ MPa/K}$	[47]
$N_{MX}$ (number density of MX precipitate)	$3 \cdot 10^{20} \text{ m}^{-3}$	[6]*
$D_{MX}$ (average diameter of MX precipitate)	37 nm	[13]
$h_{MX}$ (trapping coefficient for MX precipitates)	1	[6]*
$\tau_0$ (friction stress)	0 MPa	[72]
$\tau_p^s$ (hardening contribution of MX precipitates)	365 Mpa for 873K (600°C) 325 Mpa for 923K (650°C) 315 Mpa for 973K (700°C)	
$m$ (exponent factor)	2	[42,49,50]
$\alpha_0^{ss'}$ (saturation dislocation-dislocation interaction)	$0.7 (s = s')$ ; $0.05 (s \neq s')$	[71]*
$V$ (resolved shear stress variance)	$1000 \text{ MPa}^2$	
$\Delta G_{0,\rho}$ (zero-stress activation energy for dislocations)	2.8 eV	
$\Delta G_{0,MX}$ (zero-stress activation energy for MX precipitates)	7 eV	
$p$ (exponent parameter)	0.7	[48]*
$q$ (exponent parameter)	1.4	[48]*
$\nu_{G,MX}$ (attack frequency for MX precipitate obstacle)	$1.2 \cdot 10^{10} \text{ s}^{-1}$	[22]*
$R_e$ (proportion of edge dislocations)	10%	
$\chi$ (entropy factor)	1	[36]
$r_d$ (inner radius of dislocation control volume)	$4b$	[52]
$r_\infty$ (inner radius of dislocation control volume)	$200b$	
$\rho_{cell,0}^s$ (initial dislocation density in the cell)	$4 \cdot 10^{12} \text{ m}^{-2}$	[14,73–75]*
$\rho_{cw,0}^s$ (initial dislocation density in the cell wall)	$1 \cdot 10^{13} \text{ m}^{-2}$	[14,73–75]*
$l_\rho$ (average distance to climb for dislocation obstacle)	$100b$	
$k_1$ (material constant)	0.12	
$k_2$ (material constant)	85	
$k_3$ (material constant)	$0.5 \cdot 10^9$	
$k_c$ (material constant)	0.1	
$\lambda_{sg}$ (sub-grain size)	$0.5 \cdot 10^{-6}$	[73]
$n_0$ (annihilation strain rate sensitivity)	3.5	
$D_v^0$ (diffusion constant)	$7.87 \cdot 10^{-7} \text{ m}^2/\text{s}$	[76]
$E_m^v$ (vacancy migration energy)	0.6 eV	[76]
$g_0$ (coefficient used in Eq. 35)	1.724 eV	[76]
$g_1$ (coefficient used in Eq. 35)	$-1.2 \cdot 10^{-4} \text{ eV/K}$	[76]
$g_2$ (coefficient used in Eq. 35)	$-2.79 \cdot 10^{-8} \text{ eV/K}^2$	[76]
$g_3$ (coefficient used in Eq. 35)	$-5.93 \cdot 10^{-11} \text{ eV/K}^3$	[76]

\* Parameter estimated or back-fitted from experimental data within the range given in the listed references.